

Localization and causality for a free particle

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Abstract

Theorems (most notably by Hegerfeldt) prove that an initially localized particle whose time evolution is determined by a positive Hamiltonian will violate causality. We argue that this apparent paradox is resolved for a positive energy free particle described by either the Dirac equation or the Klein-Gordon equation because such a particle cannot be localized in the sense required by the theorems.

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1 Introduction

According to Hegerfeldt's theorem [1], “Positivity of the Hamiltonian alone [means] that particles, if initially localized in a finite region, immediately develop infinite tails.” Does this mean signals propagate faster than light [2]? Is causality in jeopardy of being overthrown, or is this theorem further evidence of cracks in the foundations of quantum mechanics? In our view, the Hegerfeldt theorem does *not* imply a failure of causality or relativity. Instead, it is a comment on the nature of quantum mechanics (but not a fatal flaw in quantum mechanics). Hegerfeldt's theorem is an “if...then” statement, and since the “then” part (immediate infinite tails) is nonsensical physics, we conclude that the “if” part of the theorem (localized wave functions) should not be realizable for a sound quantum theory. Thus Hegerfeldt's theorem really means that a logically consistent single-particle quantum theory should not allow localization. To back up this claim, we offer analyses of the free-particle Dirac and Klein-Gordon equations to show that for positive energy

solutions, the traditional definitions of particle density (or energy density for the Klein-Gordon equation) do not allow the localization required by the Hegerfeldt theorem.

We will focus our attention on the strongest version of Hegerfeldt's theorem, presented in Ref.[3], and referred to as H1. The H1 theorem obtains superluminal speeds if the probability of finding a particle outside a bounded region decays with distance at a sufficiently large exponential rate. The results derived here apply to H1 as well as to weaker versions of the theorem (where more stringent localization is needed to prove superluminal speed) [4], [5]. Our results are not directly related to localization theorems of field theory (see e.g. J.M. Knight[6]).

The building blocks of Hegerfeldt's theorem are a positive Hamiltonian, H , and a localization operator, $N(V)$, whose expectation value corresponds to the probability of finding a particle (or a particle's energy) inside a volume V . To investigate applicability of the theorem, it is natural to consider a Hamiltonian and localization operator based on the most familiar relativistic wave equations of quantum mechanics: the Dirac and Klein-Gordon equations. We will consider both these cases.

For a free particle, one can construct a positive Dirac Hamiltonian by restricting the Hilbert space of wave functions to positive energy solutions. The simplest definition of $N(V)$ is then obtained by projecting the standard Dirac probability density onto this positive-energy Hilbert space.

For the Klein-Gordon equation, the positive energy Hamiltonian is obtained by taking the square root of the Klein-Gordon equation. The absence of a positive Klein-Gordon probability density forces us to consider an alternative interpretation of the Hegerfeldt theorem. If one associates $\langle N(V) \rangle$ with the probability of finding the particle's *energy* in the region V , then $N(V)$ is positive, normalizable and well-defined. Furthermore, the interpretation of $\langle N(V) \rangle$ as the probability for finding the particle's energy in the volume V does not change the superluminal implication of the theorem.

Our basic conclusion is that H1 cannot be applied to the Dirac or Klein-Gordon equations using the $N(V)$ described above because one cannot form a sufficiently localized $\langle N(V) \rangle$ to satisfy the postulates of the theorem. We view this as a positive result, because it gives one greater confidence in the internal consistency of these cornerstones of quantum mechanics. For both the Dirac and Klein-Gordon equations, our mathematics can be summarized and simplified in terms of the momentum space wave function, $\psi(\vec{k})$. Local-

ization is inconsistent with the wave equations because

$$\begin{aligned} \textit{localization} &\Rightarrow \textit{analytic } \psi(\vec{k}) \\ \textit{wave equation} &\Rightarrow \textit{nonanalytic } \psi(\vec{k}) \end{aligned}$$

The “analytic-nonanalytic” distinction will be made precise in Sections 2 and 3, where we will discuss the Dirac and Klein-Gordon examples.

One can consider alternative forms for $N(V)$ which allow the localization needed to apply Hegerfeldt’s theorem. One famous alternative is based on the Newton-Wigner[7] position operator, which *does* satisfy the postulate of H1 (as well as weaker versions of the theorem). In our opinion, the fact that superluminal velocities would occur if the Newton-Wigner approach were valid is another argument against Newton-Wigner localization. The Newton-Wigner approach also encounters difficulty with Lorentz invariance, and particle conservation. (See Kalnay[8] and Rosenstein and Usher [9] for additional discussion).

We need to be precise about the meaning of “localization.” In H1 superluminal speed was proved when a particle was exponentially localized so that the probability of finding the particle outside a sphere of radius R was bounded by $\bar{A}^2 \exp(-2\gamma R)$, with $\bar{A} < \infty$ and $\gamma > m$. We use units where $\hbar = c = 1$, so the particle’s mass m corresponds to the inverse of its Compton wave length $\lambda = \hbar/(mc)$. We take this bound as our definition of localization and apply it in Sections 2 and 3. The final section includes some comments and a brief discussion of other work. In particular, we acknowledge the importance of work by Thaller [10] in our derivations.

2 Dirac Equation

Hegerfeldt’s theorem applies to systems with a positive Hamiltonian, but the Dirac equation has both positive and negative eigenvalues. However, for free particles, the Hilbert space \mathcal{H} of solutions to the Dirac equation is the sum of positive energy and negative energy Hilbert spaces.

$$\mathcal{H} = h_+ + h_- \tag{1}$$

The Dirac free-particle Hamiltonian is well-defined and positive on h_+ .

The Dirac equation allows the construction of a particle current 4-vector, whose time-like component is a probability density

$$\rho(\vec{r}, t) = \sum_{i=1}^4 \psi_i^*(\vec{r}, t) \psi_i(\vec{r}, t) \quad (2)$$

where the sum is over spinor components. (In the notation of QED, this is written as $\rho = \bar{\psi} \gamma_0 \psi$.) Associated with this probability density is an operator $N(V)$ which gives the probability that a particle is within a volume V .

$$N(V) = I_4 P(V) \quad (3)$$

where $P(V)$ is the projection onto the volume V

$$P(V) = \begin{cases} 1 & \vec{r} \in V \\ 0 & \vec{r} \notin V \end{cases} \quad (4)$$

and I_4 is the unit 4×4 matrix which operates on the 4-component spinors. In the full Hilbert space of 4-component solutions, particles can be localized. For example, one can pick wave functions which vanish outside a finite region of space. But these localized states do not lie in the positive energy space h_+ , and projecting them into h_+ yields non-localized wave functions. It is this delocalization which makes the application of Hegerfeldt's theorem impossible.

The natural generalization of $N(V)$ to h_+ is

$$N(V)_+ = P_+ N(V) P_+ \quad (5)$$

where P_+ is the projection from \mathcal{H} onto h_+ . Then for any wave function $\psi \in h_+$, $P_+ \psi = \psi$ and

$$\langle \psi, N(V)_+ \psi \rangle = \langle \psi, N(V) \psi \rangle \quad (6)$$

gives the probability that a positive energy particle is within the volume V . Thus when working with wave functions in h_+ , one can use the definition of Eq. (2) and omit the subscript on $N(V)$.

To apply Hegerfeldt's theorem as described in H1, one must first exhibit a normalized wave function in h_+ which is localized so that [3]

$$\langle \psi, N(B_r) \psi \rangle > 1 - \bar{A}^2 \exp(-2\gamma r) \quad (7)$$

where B_r is a sphere of radius r and $\gamma > m$. This inequality can be satisfied only if there is a wave function in h_+ , each of whose components satisfies the condition

$$|\psi_i(\vec{r}, 0)| < A \exp(-\gamma r) \quad (8)$$

for all \vec{r} and a finite A . This bound on $\psi_i(\vec{r}, 0)$ implies a range of analyticity of the Fourier transform of the wave function components given by

$$\psi_i(\vec{k}) = \frac{1}{(2\pi)^{3/2}} \int \exp(-i\vec{k} \cdot \vec{r}) \psi_i(\vec{r}, 0) d^3r \quad (9)$$

Localization means each $\psi_i(\vec{k})$ is an analytic function of the vector components of \vec{k} in the complex-plane strip characterized by

$$|\text{Im}(\vec{k})| \leq m \quad (10)$$

Rather than presenting a proof of this analytic property, we illustrate the structure of $\psi_i(\vec{k})$ with a simple example. Assume a $\psi_i(\vec{r}, 0)$ is minimally localized, so that it takes on the value of its upper bound in Eq. (8). Then the Fourier integral (obtained most simply in spherical coordinates where $d^3r = 2\pi r^2 d(\cos \theta) dr$ and $\vec{k} \cdot \vec{r} = kr \cos \theta$) gives

$$\psi_i(\vec{k}) = \frac{A}{(2\pi)^{3/2}} \frac{8\pi\gamma}{(k^2 + \gamma^2)^2} \quad (11)$$

which is analytic for $|\text{Im}(\vec{k})| < \gamma$, and since $\gamma > m$ we obtain the condition of Eq. (10). If the wave function is more strongly localized, so the magnitude of $\psi_i(\vec{r}, 0)$ is decreased, the range of analyticity of $\psi_i(\vec{k})$ can only increase. A formal analyticity proof is based on Theorem IX.13 of Reed and Simon [11].

The Dirac equations yields the opposite conclusion on the analyticity of wave functions. The requirement of positive frequency means the four components of the wave function are not all independent. For spin-polarization $\vec{\sigma}$, the components of the momentum space wave function must satisfy the condition [10]

$$\begin{pmatrix} \psi_3(\vec{k}) \\ \psi_4(\vec{k}) \end{pmatrix} = \frac{\vec{k} \cdot \vec{\sigma}}{\sqrt{m^2 + k^2} + m} \begin{pmatrix} \psi_1(\vec{k}) \\ \psi_2(\vec{k}) \end{pmatrix} \quad (12)$$

The branch cut in $\sqrt{m^2 + k^2}$ at $k = im$ means all four components $\psi_i(\vec{k})$ cannot be analytic when \vec{k} is imaginary with magnitude m , and this is inconsistent with Eq. (10).

This analysis of the wave function's analytic structure shows that Hegerfeldt's theorem does not apply to positive energy free particles described by the Dirac equation (with the traditional probability density) because these particles cannot be described by localized wave functions. The exponential tail required of positive energy solutions to the Dirac equation decays too slowly to allow application of the theorem of H1.

3 Klein-Gordon Equation

The interpretation of a single spin-zero particle described by the Klein-Gordon equation presents different problems. A positive probability density cannot be defined (even for a free particle). However, one can consider a modification of Hegerfeldt's result which uses the particle's energy density instead of its probability density as the basis for constructing an $N(V)$. Since relativity also limits the propagation speed of energy to be less than the speed of light, the potential contradiction of quantum mechanics and relativity is still an issue.

The Klein-Gordon equation is

$$-\frac{\partial^2 \psi}{\partial t^2} = -\nabla^2 \psi + m^2 \psi \quad (13)$$

The positivity assumption means the only allowed solutions are linear combinations of positive frequency plane wave states of the form

$$\psi_k(\vec{r}, t) = \exp(i\vec{k} \cdot \vec{r} - i\omega(k)t) \quad (14)$$

with

$$\omega(k) = +\sqrt{k^2 + m^2} \quad (15)$$

Thus the Klein-Gordon equation restricted to positive frequencies can be written as

$$i\frac{\partial \psi}{\partial t} = \sqrt{-\nabla^2 + m^2} \psi \quad (16)$$

where the meaning of the positive energy operator on the right is obtained from the Fourier transformed expression for ψ .

As is well known from the history of the Klein-Gordon equation, one cannot easily justify $\psi^* \psi$ as a probability density. (However, it is related to the

Newton-Wigner[7] approach to localization.) The standard Klein-Gordon density is the “charge density”

$$\rho_c = \frac{i}{2} \left(\psi^* \frac{\partial \psi}{\partial t} - \psi \frac{\partial \psi^*}{\partial t} \right) \quad (17)$$

However, ρ_c is not always positive, even for the positive frequency free-particle solutions to the free-particle Klein-Gordon equation.

Because we cannot identify a probability density with acceptable physical properties, we propose that the Klein-Gordon energy density is the appropriate way to characterize particle localization. This energy density is proportional to

$$T(\vec{r}, t) = |\vec{\nabla} \psi|^2 + \left| \frac{\partial \psi}{\partial t} \right|^2 + m^2 |\psi|^2 \quad (18)$$

We can normalize ψ so that the integral of $T(\vec{r}, t = 0)$ over all space is unity (in a fixed coordinate system). Furthermore application of the Klein-Gordon equation (for a free particle with positive frequencies) shows that this integral cannot vary in time, so a convenient normalization gives

$$\int T(\vec{r}, t) d^3r = 1 \quad (19)$$

for any t . With this normalization, we define an operator $N(V)$ with $0 \leq N(V) \leq 1$ which can be interpreted as the probability that the particle’s energy is confined within the volume V , because

$$\langle \psi, N(V) \psi \rangle = \int_V T(\vec{r}, t) d^3r \quad (20)$$

Since the momentum operator $-i\vec{\nabla}$ and the operator $\sqrt{-\nabla^2 + m^2}$ of Eq. (16) are Hermitian, the $N(V)$ of Eq. (20) for positive energy states is

$$N(V) = \sqrt{-\nabla^2 + m^2} P(V) \sqrt{-\nabla^2 + m^2} - \vec{\nabla} \cdot (P(V) \vec{\nabla}) + m^2 P(V) \quad (21)$$

where $P(V)$ is the projection onto the volume V , as defined in Eq. (4).

If $\langle \psi, N(V) \psi \rangle$ could be exponentially localized, Hegerfeldt’s theorem would mean a Klein-Gordon particle’s energy density could propagate faster than light. We show that this is impossible following essentially the same reasoning as was used for the Dirac equation. Using Eqs. (18, 20) localization

would mean both $\psi(\vec{r}, 0)$ and $\partial\psi(\vec{r}, 0)/\partial t$ should be constrained by the exponential bound of Eq. (8). However, as with the Dirac equation, the bounds impose an analytic structure on the Fourier transform of the wave functions. Using standard relativistic notation, we write

$$\psi(\vec{r}, t) = (2\pi)^{-3/2} \int \left(\frac{\hat{\psi}(\vec{k})}{\omega(\vec{k})} \right) \exp(i\vec{k} \cdot \vec{r} - i\omega(k)t) d^3k \quad (22)$$

where $\hat{\psi}(\vec{k})$ is the “momentum-space wave function.” The inverse Fourier transform of Eq. (22) gives

$$\frac{\hat{\psi}(\vec{k})}{\omega(\vec{k})} = (2\pi)^{-3/2} \int \psi(\vec{r}, 0) \exp(-i\vec{k} \cdot \vec{r}) d^3r \quad (23)$$

Differentiating Eq. (22) with respect to time and then taking the inverse Fourier transform gives

$$\hat{\psi}(\vec{k}) = (2\pi)^{-3/2} \int i \frac{\partial}{\partial t} \psi(\vec{r}, 0) \exp(-i\vec{k} \cdot \vec{r}) d^3r \quad (24)$$

If both $\psi(\vec{r}, 0)$ and $\partial\psi(\vec{r}, 0)/\partial t$ satisfy the localization condition of Eq.(8), then both $\hat{\psi}(\vec{k})/\omega(k)$ and $\hat{\psi}(\vec{k})$ must be analytic functions of the components of \vec{k} in the strip of the complex plane described by Eq. (10). This is not consistent with the branch cuts in $\omega(k)$ at $k = \pm im$ which are displayed in Eq. (15).

The Klein-Gordon wave equation combined with our definition of $N(V)$ gives the momentum space wave function an analytic structure which prevents the localization required by H1. Thus Hegerfeldt’s theorem cannot prove superluminal energy propagation for free positive energy particles described by the Klein-Gordon equation.

4 Comments

An alternative way around the paradox suggested by Hegerfeldt’s theorem is based on physical arguments. Berestetskii, Lifshitz and Pitaevskii [12], [13] point out that single-particle quantum mechanics becomes inadequate (e.g. pair creation) whenever an experiment is done to show that a particle is localized in a region smaller than its Compton wave length. This idea

was pursued further by Kaloyerou [14]. Yndurain [15] and other have used the problems associated with localization as one of the motivations for abandoning quantum mechanics for field theory. While we do not question the arguments for field theory, we do feel that the localization problem continues to deserve attention. Even if ordinary relativistic quantum mechanics is not a fundamental description of nature, the applicability and limitations of single-particle theories are of practical importance.

An early form of Hegerfeldt's theorem has been known for many years, and many have considered its consequences [2], [16], [17], [18]. We are not the first to suggest that particles cannot be localized. Perez and Wilde [19] suggested that particles could be only "essentially localized" [20], [21]. Thaller [10] noticed that a Dirac particle could not be so strictly localized that its wave function vanished outside a finite region. Our results are an extension of Thaller's.

The non-localization of Dirac electrons may appear to contradict the result of Bracken and Melloy, who in the paper "Localizing the relativistic electron" obtain a sequence of states whose position uncertainty can be made arbitrarily small [16]. The results are not inconsistent. Since the Bracken-Melloy sequence is not a Cauchy sequence, the localized pointwise limit function cannot be treated as a solution to the Dirac equation.

The problem with the positivity of the Klein-Gordon charge density ρ_c has been frequently discussed when an external potential is added to the Klein-Gordon equation. Sometimes a negative ρ_c is (dubiously) attributed to strong-field effects (see for example Ref. [22]).

Our suggestion that the energy density is an appropriate alternative to the probability density is not new. This situation is commonly acknowledged for the photon. For example, Akhiezer and Berestetskii [23] comment that "... the localization of a photon in a region smaller in order of magnitude than a wavelength has no meaning, and the concept of probability density for the localization of a photon does not exist. ... In practice, it is often sufficient (instead of the equation of continuity for the probability density) to utilize the equation of continuity for the energy density." We claim that these same comments should apply to a Klein-Gordon particle, except the size of the position uncertainty is the particle's Compton wave length rather than the photon's classical wave length. We admit to a prejudice here. Some argue (e.g. Ref. [24]) that a photon does have a position operator. If such an operator exists, it is certainly not simple.

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